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Summary Report for Fiscal Year 1993

USDOE/OTD TTP No. AL131004:

Multi-Spectral Nuclear Logging

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I. EXECUTIVE SUMMARY

Certain nuclear geophysical borehole logging techniques are capable of identifying and mapping specific nuclides in the rock or soil through which a borehole passes. Thus, such techniques are potentially useful for environmental restoration (ER), where characterization of contaminated sites is required before cleanup can begin and long-term monitoring is needed for many years after either cleanup or stabilization has been accomplished. Nuclear borehole logging techniques have advantages and disadvantages that tend to be complementary to those of physical sampling and can help address the drawbacks of physical sampling. These drawbacks include high costs, lengthy delays in obtaining results of analyses from overburdened laboratories, under sampling, sample handling problems, and ambiguity in long-term monitoring.

One of the most potentially useful nuclear geophysical logging techniques for contaminant mapping is neutron-induced spectral gamma-ray (Multi-Spectral) logging. Neutron-induced SGR techniques measure gamma-ray energy spectra during and/or after irradiation of the borehole environment by neutrons. As such, they are analogous to laboratory techniques such as neutron activation analysis. Neutrons interact with nuclei in a variety of ways, such as inelastic scattering, prompt capture, and activation, to produce gamma rays that enable those specific nuclides to be positively identified under favorable conditions. Detectable contaminants include chlorine, a component of many organic contaminants, as well as heavy metals and other materials. The physics behind this technique is generally well understood and it is known that it can identify many radioactive and non-radioactive nuclides. The key question is thus: what is the detection threshold for each of those nuclides for the range of conditions that the borehole logging system will encounter? This project is focused on answering that question for a state of the art Multi-Spectral logging system. The project is a cooperative effort under three separate but related TTPs: TTP No. 131004 from Los Alamos National Laboratory, which includes effort by Lawrence Livermore National Laboratory and others, TTP No. AL931001 from DOE/GJPO produced by RUST Geotech, a DOE contractor, and TTP No. AL031001 produced by the U. S. Geological Survey (USGS). This Annual Summary Report is for TTP No. AL131004. Los Alamos has primary responsibility for computer simulations and interpretation theory, while RUST Geotech has primary responsibility for experiments and field work. Geotech and the USGS share hardware development responsibilities.

Computer modeling of nuclear processes is widely used in nuclear engineering applications such as radiation shielding design and criticality studies, and has also been used to help design and understand nuclear borehole logging instruments. For that latter application, computer modeling codes are benchmarked and validated using experimental data from a few physical models. Then, computer simulations are used to study numerous sets of conditions including a variety of instrument designs, all of which would be difficult or prohibitively expensive to do using any other approach. The statistical simulation approach commonly used for nuclear transport calculations are called "Monte Carlo" models because their execution is guided by repeated throws of computerized dice, i.e., a numerical random number generator. These random numbers are used, along with probability functions representing each of the categories of events that can occur, to determine the flow of the simulation. Nuclear processes are inherently random and can be very accurately simulated by the Monte Carlo approach.

As part of this project, we have evaluated available Monte Carlo codes and selected two to work with. One is MCNP, written and maintained at Los Alamos National Laboratory. The other is a program written and maintained at North Carolina State University in the Nuclear Engineering Department. MCNP is primarily intended for shielding and criticality calculations and it is the state of the art code for those applications but we have found it to be somewhat intractable for our particular application because it has not been optimized for simulating neutron-induced gamma-ray spectroscopy problems. The North Carolina State University program is available at moderate cost but is supported at a low level relative to MCNP. The design of this program offers some advantages over MCNP for this application, so we are testing it as well. Much of our work in FY-93 has been directed towards evaluating and improving these two Monte Carlo codes to make them more usable for this application.

At the time that we received funding for this project, our plan as set forth in the TTPs was for RUST Geotech (DOE/GJPO) and the U.S. Geological Survey to put together a test system capable of gathering data that could be used to evaluate and benchmark the computer simulation models. At about that same time we became aware that there was a newly formed small company that had the capability to make those experimental measurements. We decided that we should use an industrial partner such as this company to obtain the benchmark data. RUST Geotech began the paperwork that they felt was required to hire a contractor to run the experiments. This process proved to be very slow, and the USGS did not receive their FY-93 funding until the last few weeks of FY-93. Because of these delays it became evident that we would need to identify another source of benchmark data. Environmental Measurements Corporation (EMC) supplied us with two experimental spectra.

The experimental data used for benchmarking MCNP in FY-93 was obtained in the Atlas Wireline Services glass plate model. This model consists of glass plates stacked with spacers to provide simulated porosity, and includes a steel-cased and cemented borehole. The borehole was filled with a sodium bromide solution, and the voids between the glass plates were filled with a saline solution. EMC provided some schematics of the nuclear well-logging instrument package and as much detail as possible was included in the MCNP geometry specification for the instrument, which uses a 14-MeV pulsed neutron generator and a hyper-pure germanium (HPGe) detector.

After installation, debugging and testing of MCNP, we ran several long simulations. The best simulation was on an HP-735 with 112 Mbytes of RAM. This simulation used 14,500 minutes of CPU time, tracking 3.596×10^7 source neutrons. All capture gamma-ray lines observed experimentally are reproduced by MCNP.

The primary differences between the experimental data and the simulated spectra result from the unavailability of cross-section data for germanium, which makes the HPGe detector response difficult to model. Since the efficiency of the detector cannot be reproduced, there is no generation of escape peaks; also, MCNP is unable to simulate the gamma rays from Ge(n,γ) reactions, seen experimentally below about 1.5 MeV. The MCNP detector response is the response that would be obtained by a 'perfect' detector, accurately detecting all gamma rays entering its space and generating no escape peaks. Los Alamos group X-6 is currently processing Ge cross-sections for us and these should be available early in 1994.

While MCNP simulates a perfect detector, the experimental data were taken with a relatively small detector. For example, the MCNP simulation shows nine distinct Cl lines that do not appear in the experimental data. The experimental spectra are dominated by the double and single escape peaks rather than the primary energy peak for each gamma ray. This makes the identification of the appropriate nuclides and the estimation of concentrations more difficult. It is easy to see that the perfect detector response of MCNP leads to the identification of more capture gamma-ray lines than the experimental data.

The simulation of the EMC glass-plate experiment indicates that MCNP can be used to simulate experimental results with several important constraints. For this application, MCNP is primarily limited by the availability and quality of the neutron cross-sections. Some neutron cross-sections are unavailable due to lack of experimental data, while others are unavailable because existing data have not been processed into the MCNP format. The unavailability of cross-sections for some environmental contaminants, due to a lack of experimental data, is a problem that is difficult to address because limited time and budget, and because of the ongoing cutbacks in our national nuclear experimental facilities. We are having some important cross-section data sets that are available as experimental data converted into the proper MCNP format. We are also commissioning some minor modifications to the code. Finally, we hope to improve the accuracy of the photon-production spectra in MCNP. These steps should contribute significantly toward making the simulations more reliable and accurate.

II. INTRODUCTION

This Annual Summary Report deals with both technical issues and administrative issues. Administrative issues are reviewed in Appendix A, Budget and Schedule. Most of the remainder of the report deals with technical issues.

A. Overview

Geophysical borehole logging techniques are used for the in-situ determination of subsurface chemical, physical, geological and hydrological parameters. This project deals with the application of nuclear logging techniques to map environmental contaminants along boreholes. Most existing nuclear borehole logging techniques were developed for use in the petroleum industry[1-2] or for uranium exploration and uranium prospect evaluation[3], and thus have not been optimized for this new and technically challenging application. Several nuclear techniques are currently in use, or being evaluated, for contaminant mapping. Because even small concentrations of some contaminants can be of concern, the key question in such evaluations is: what is the detection threshold for a given contaminant for the range of conditions that the borehole instrument will encounter?

The environmental problems within the United States Department of Energy (DOE) complex of laboratories and production facilities have received widespread attention in the press in recent years. The DOE Environmental Restoration (ER) Program faces the task of identifying and mapping a large number of different contaminants in landfills, surface disposal areas, spill sites and subsurface contaminant plumes across the complex. Because of pressure from the public and from regulatory agencies, site characterization is proceeding rapidly at DOE sites using existing technology, mainly physical sampling with extensive laboratory analyses. Nuclear borehole logging techniques, which have advantages and disadvantages that tend to be complementary to those of physical sampling, are capable of identifying and mapping specific nuclides in the rock or soil through which a borehole passes[4] and can help address the drawbacks of physical sampling in certain cases.

B. Why *in-situ* measurements?

There is no doubt that the analysis of physical samples extracted from boreholes will remain the primary method of characterizing the borehole environment for the foreseeable future. However, direct measurements in boreholes can and should also play an important role, the extent of which remains to be determined. Borehole logging techniques have advantages and disadvantages that are generally complementary to those of physical sampling and can be used to address the problems that are often associated with physical sampling.

C. Potential drawbacks of physical sampling

The potential drawbacks of physical sampling include: (a) high costs, (b) lengthy delays in obtaining results of analyses from overburdened laboratories, (c) under sampling, (d) sample handling problems, and (e) ambiguity in long-term monitoring. These are discussed below.

1. High costs

   The cost of drilling a borehole in contaminated soil at Hanford is reportedly in the range of $3000 to $6000 per meter or, say, $150,000 for a 30 m borehole. Most of that cost reflects the overhead associated with procurement, operations, and compliance with all regulations. Given that investment, obviously we would like to maximize the information from each borehole. A representative sampling scenario for a site characterization borehole might be to extract and analyze 20 samples at 1.5 m intervals at a cost of, perhaps, $5000 per sample or $100,000 for this 30 m borehole; the authors have heard costs reported as high as $250,000 for a full suite of laboratory analyses on one sample (again, largely reflecting overhead costs -- highly contaminated samples are expensive to extract, handle and analyze). Techniques are needed that can reduce the cost of the site characterization process, and nuclear borehole measurements have that potential. If the 30 m borehole described above is cased with sealed casing so that contamination of the equipment is unlikely, it is reasonable to estimate that it could be logged and the data processed for between $1000 and $10,000 as part of an overall logging program, a small fraction of the total cost of the entire borehole investigation.

2. Lengthy delays

   Long turnaround times for laboratory analyses of samples can be a problem; turnaround times for some sample analyses for DOE sites are reportedly approaching one year at this time. Nuclear logging techniques can yield same-day or even real-time results.

3. Under sampling

   Although the accuracy of a single laboratory sample analysis may be quite high, using those laboratory results to infer the true three-dimensional distribution of contaminants in the ground involves a number of assumptions and a statistical leap of faith. Potential errors associated with under-sampling, greatly reduce the benefits that might be expected from the accuracy advantages of sample analyses.

Exacerbating this problem is the fact that the extent of any sampling program is constrained by the high costs described above. To take an arbitrary example, assume 30 m deep boreholes are drilled on a 30 m grid such that each borehole represents a cube of material 30 m on a side, and that twenty samples, each with a volume of 50 cm^3, are extracted from each borehole and analyzed. The total sample volume analyzed from these boreholes represents roughly one part in 30,000,000 of the total volume of material being characterized. In contrast, logging the same boreholes with, say, the passive spectral gamma-ray technique represents a volume of investigation roughly equivalent to a 30 m long cylinder 30 cm in radius, or approximately one part in 3000 of the volume being characterized. These figures can be reworked using other assumptions, but characterization plans involving physical sampling alone are prone to under sampling. Since geology and contaminant migration paths are rarely uniform, under sampling can greatly reduce data confidence.

4. Sample handling problems

   Problems associated with extraction of physical samples from boreholes and repeated handling of those samples are well known. As a brief illustration, take the relatively straightforward task of analyzing for gamma-emitting contaminants using gamma-ray spectrometry. Physical sampling in boreholes involves coring, sidewall sampling, or other techniques for extracting the samples, techniques that can alter the physical properties of the samples or produce biased samples depending on the physical properties of the material. Samples must be removed from the sampling device, handled, packaged, labeled, and transported to a sample preparation facility, There, the samples are crushed, split, packaged, labeled, handled and shipped to an analysis lab. There they are handled, dried, packed tightly in analysis containers having the geometry and construction required for the particular laboratory spectrometer, labeled, weighed and, finally, analyzed. The results are then sent to the site characterization team for incorporation into their database. Any process involving this many steps and handling by this many people is susceptible to numerous sources of error.

5. Ambiguity in long-term monitoring

   Physical sampling plays a useful role in site characterization, albeit constrained by high costs. For post-closure monitoring, however, physical sampling is less useful. If you extract and analyze samples repeatedly and find that the results are significantly different from earlier samples, you do not know if the environment has changed or if the material you are analyzing is simply different from the earlier samples. In the case of long-term monitoring for contaminants, in-situ nuclear logging measurements offer great advantages in terms of continuous coverage, large sample volume, and the ability to run repeat measurements in the same borehole year after year at reasonable cost. Once the borehole is cased, extraction of further samples becomes difficult, but most nuclear measurements can be made through casing. Thus, nuclear logging techniques are very well suited for long-term monitoring, allowing the same boreholes to be scanned at regular time intervals for as many years as required.

6. Reduced costs and enhanced data confidence

   Los Alamos and Lawrence Livermore National Laboratories adapted an existing nuclear logging technique, neutron-induced spectral gamma-ray logging, at the Nevada Test Site to analyze the rock for the presence of carbonates. The technique is essentially a less sophisticated version of the Multi-Spectral technology under development in this project, which will be described later in this report. At this point it is useful to consider this example as a case study in achieving the goal of reduced costs and enhanced data confidence using nuclear logging techniques.

   When an underground nuclear test is conducted, the presence of carbon is potentially hazardous because it can combine with oxygen to form gaseous CO_2. When the cavity cools, most materials condense out but CO_2 remains a gas, possibly under sufficient pressure to drive a delayed leak of radioactive materials to the surface. In the past, Los Alamos National Laboratory used sidewall sampling, at a cost of up to $50,000 per borehole, to obtain samples for carbonate analysis. Even with that costly sampling program, less than one-billionth of the cavity material was sampled, and the results were biased by the physical properties of the material.

   In a joint project, Los Alamos and Lawrence Livermore National Laboratories developed new calibration factors, quality control techniques, and data reduction techniques to allow us to use an existing commercial multi-spectral logging service to analyze the rock for the presence of carbonates[5,6]. The logging data are less accurate than sample analyses, but give a continuous record of carbon distribution with depth, analyzing some 10^4 times the volume of rock analyzed by physical sampling, for about $1000 per borehole as part of a larger borehole logging contract.

   As a test, we logged an existing borehole that had been extensively sampled and found a potentially dangerous 12 m thick zone of high carbon content that had been missed entirely by the sampling; this zone was confirmed by subsequent additional sampling. By combining a reduced sampling program with nuclear borehole logging, we can achieve greatly enhanced data confidence at a reduced cost. Such a win-win result may be obtained for some contaminants in ER by applying appropriate nuclear borehole logging techniques.

D. Need for this technology

Techniques for mapping contaminants *in-situ* with borehole instrumentation are applicable directly or indirectly a number of needs listed in the FY-94 CMST-IP Request for Proposals, as described below.

1. Direct applicability

   Need 1.2: Field analysis equipment for real-time results. The techniques proposed here will produce same-day analyses of the material along entire boreholes.

   Need 2.2: Significantly improved analytical methods or sensors. This technology will help speed up site characterization while reducing the load on analytical laboratories and reducing costs.

   Need 3.2: Improved in-situ measurements of subsurface properties. This technology represents a method for analyzing boreholes for gamma-emitting contaminants that is literally better, faster, cheaper and safer than existing technology.

2. Indirect applicability

   Need 1.1: Sensors instrumentation and sampling probes for deployment by cone penetrometers or other minimally intrusive methods for determination of ... radionuclides. The data processing techniques developed to make nuclear borehole measurements quantitative will be needed for any similar nuclear measurements made now or in the future using cone penetrometers.

   Need 1.3: Statistically guided sampling and data quality assurance tools. The key goal of this proposal is to achieve regulatory acceptance of this in-situ analysis technique in the same way that laboratory analyses of core samples are now acceptable. The assumptions inherent in the techniques proposed here are no more questionable than those inherent in sampling and laboratory analyses, and the advantages are clear.

III. THEORY

For FY-93, this project was focused entirely on *neutron-induced* spectral gamma-ray borehole logging, or *active* spectral gamma-ray logging. However, for FY-94, the Los Alamos part of the project has been broadened to include development of data processing techniques for *passive* spectral gamma-ray logging. Because these two techniques are closely related and are now both part of this project, they will both be discussed here.

A. Passive spectral gamma-ray techniques

Passive spectral gamma-ray (SGR) logging can detect and identify the artificial gamma-emitting nuclides that are found in the ground at some DOE waste sites, as well as natural gamma-emitting nuclides found in most rocks and soils. The detectors used in these instruments are usually low energy-resolution scintillators{7-9}, but a few instruments containing high energy-resolution, solid-state cryogenic detectors have been built and are in use today{10,11}. In the case of low energy-resolution detectors, full spectral processing{12} is generally needed to identify specific nuclides present in the vicinity of the borehole because the broad photopeaks from different gamma-ray energy lines overlap. In the case of high energy-resolution detectors, overlapping peaks pose much less of a problem, but automatic picking of specific characteristic energy lines from the complicated spectrum is still desirable{13,14}.

Passive SGR logging is an extremely sensitive indicator of gamma-emitting nuclides in the ground. For example, under typical conditions the technique can detect ^{214}Bi, a daughter of ^{238}U, in concentrations on the order of 1 part in 10^{14} by weight. We estimate that a detection threshold on the order of 0.1 pCi/g for ^{137}Cs is achievable using passive SGR logging; by comparison, typical background concentrations are an order of magnitude higher while screening action levels are typically two orders of magnitude higher.

Although passive SGR borehole logging is underutilized in ER work, it is being used successfully at the DOE Hanford site to identify a number of gamma-emitting contaminants such as ^{137}Cs and ^{60}Co in-situ. While the technique can be very accurate in identifying which contaminants are present, especially when a high energy-resolution detector is used, the data are not proportional to the concentrations of contaminants at a given depth except in very thick, uniform zones{15}. Because of this lack of a quantitative basis, the current use of this technique in the DOE ER program is more limited than would otherwise be the case. However, data processing techniques have been developed for passive SGR logging, particularly for uranium exploration applications, that can convert the qualitative logs to quantitative concentration profiles for individual nuclides within limitations imposed by well understood sources of error{16-18}. The application of such data processing should make passive SGR logging acceptable to regulators as a replacement for most laboratory analyses for gamma-emitting contaminants along boreholes; this could yield savings of millions of dollars at

DOE sites where gamma-emitting contaminants are a concern. These data processing techniques are briefly discussed later in this report.

Regulatory agencies require contractors at the DOE Hanford site to run passive SGR logs in each borehole to search for gamma-emitting contaminants. Other DOE sites, such as Los Alamos and Savannah River, have also identified the need to map gamma-emitting contaminants along boreholes, and passive SGR borehole logging techniques will be applied at those sites as well. Internationally, workers evaluating and cleaning up nuclear accident sites such as Chernobyl could eventually be major users of this technology. In the case of long-term monitoring for gamma-emitting contaminants, there is no reasonable substitute for in-situ passive SGR measurements. The advantages of continuous coverage, large sample volume, sensitivity and accuracy, combined with the ability to run repeat measurements in the same borehole year after year at reasonable cost, yield a monitoring tool that is generally superior to all other technologies.

B. Neutron-induced spectral gamma-ray techniques

Neutron-induced spectral gamma-ray techniques use the same detector types as the passive techniques described above, with the addition of a neutron source to produce gamma rays from nuclides that would not naturally gamma emitters. In other words, neutron-induced SGR techniques measure gamma-ray energy spectra during and/or after irradiation of the borehole environment by neutrons. As such, they are analogous to laboratory techniques such as neutron activation analysis. Neutrons interact with nuclei in a variety of ways, such as inelastic scattering, prompt capture, and activation, to produce gamma rays having energies that will enable specific nuclides to be positively identified under favorable conditions. Detectable contaminants include chlorine, a component of many organic contaminants, as well as heavy metals and other materials.

Energetic neutrons leaving the detector undergo a number of interactions with atomic nuclei, losing energy with each interaction. With each interaction, there is a finite probability that the reaction will lead to the production of one or more gamma rays. The probability of such a reaction is determined by the cross section of the nuclide for that reaction at that neutron energy. Eventually, neutrons that are not captured (in most cases this is the vast majority of neutrons) will reach thermal energy, an average energy of approximately $E_n=2.5\times10^{-8}$ MeV, where the neutron is as likely to gain energy as to lose energy from a given interaction. At thermal energies, capture cross sections are generally much greater than at higher energies, and the neutron is more likely to be captured by a nucleus. Each particular nuclide emits a unique set of discrete energy gamma rays from this capture reaction. The intensity, or area under the peak in the spectrum, of the gamma rays from a given reaction is related to the concentration for that nuclide.

While neutron-induced SGR techniques are capable of detecting and identifying many different nuclides, the technique is considerably more challenging technically than passive SGR because many materials in the vicinity of the neutron source become gamma emitters, not just the contaminants of concern. It is difficult to identify trace levels of contaminants against this background. The key goals of this project are to estimate and optimize detection thresholds for contaminants of concern for state of the art instrumentation.

As in the case of the passive SGR systems discussed above, the detector may be a high energy-resolution, solid-state cryogenic detector or a low energy-resolution scintillator. The logging instrument may contain a radiochemical source or a neutron generator. Radiochemical neutron sources have some technical advantages over neutron generators including the advantage of a source flux limited only by safety concerns. Safety, however, is a significant limitation. High-energy, high-intensity neutron sources are relatively difficult to shield and handle, and there is sometimes a resistance by regulators to putting such sources into boreholes because of the dangers of source capsule leakage or loss of the borehole instrument package due to borehole collapse. That resistance can only be expected to increase in the future.

While pulsed neutron sources do not present the safety and handling challenges of radiochemical sources, some contain several curies of tritium. Unfortunately, source flux from pulsed neutron sources can vary from burst to burst, complicating the job of calculating absolute elemental concentrations[5]. Radiochemical neutron sources, on the other hand, generally have known source intensity. This may allow elemental concentrations to be expressed directly rather than as a ratio of concentrations as is commonly the case with pulsed sources.

A number of neutron-induced SGR borehole systems have been developed for both commercial and experimental purposes. The ones described here do not constitute a complete list.

1. Low energy-resolution systems

   Pulsed neutron spectral gamma-ray borehole logging systems based on low energy-resolution scintillation detectors are in routine use in the petroleum industry[19-23]. One typical system of this type emits a 10 microsecond burst of 14 MeV neutrons from a generator tube, followed by 40 microseconds during which the tube is turned off. This cycle is repeated 20,000 times per second; other timing schemes are also used. Gamma rays detected during the neutron burst are predominantly from inelastic interactions while gamma rays detected following the burst are predominantly from prompt capture events. Thus, with suitable time gating and spectral processing, these petroleum logging systems measure two types of low energy-resolution gamma-ray spectra: inelastic and capture. As in the case of passive low energy-resolution SGR logging, full spectral processing is generally needed to identify specific nuclides.

In addition to the petroleum logging systems described above, CSIRO (Commonwealth Scientific and Industrial Research Organization, Australia) has experimented with low energy-resolution systems using ^{241}Am-Be and ^{252}Cf sources for a variety of borehole applications[24].

2. High energy-resolution systems

   Several prototype pulsed-neutron induced SGR logging systems based on high energy-resolution cryogenic gamma-ray detectors have been developed and tested. High energy-resolution is a great advantage for contaminant analysis, but these detectors tend to be inefficient, requiring relatively long counting times.

   The U. S. Geological Survey developed and evaluated a borehole logging system using a ^{252}Cf source and a Ge(Li) detector[25-27]. Schlumberger developed a prototype high energy-resolution system that could use a ^{252}Cf source or a pulsed source for test and evaluation purposes[28]. The Schlumberger system has been evaluated in various areas and used in the Continental Deep Drilling Project[29] but has not been commercialized. ARCO developed an experimental high energy-resolution system with a pulsed neutron source for experimental work in the petroleum industry[30]; this system is currently owned and operated by Environmental Measurements Corporation.

   During the DOE National Uranium Resource Evaluation (NURE) Program, a high energy-resolution system (the "Multi-Element" system) was developed for the in-situ identification of minerals associated with uranium deposits[31-36]. It is currently being evaluated at the DOE Sandia Mixed Waste Landfill Integrated Demonstration. The objective of the MWLID work is to demonstrate the performance of the neutron activation logging system in its current configuration and to develop an improved understanding of that system using computer simulations.

C. Calibration and data correction

As a logging instrument approaches the center of a thick zone of uniform composition (greater than a meter or so), the instrument response reaches a constant value such that increasing the thickness of the zone will not change that value significantly. In principle, the instrument response in a thick zone can be corrected by multiplicative and additive calibration and correction algorithms for non-standard borehole conditions such as casing, borehole fluid type, or borehole diameter different from the calibration conditions, to yield an accurate estimate of the property that the instrument is intended to measure. This is not the case for thinner radioactive zones; thin zone response will be discussed later in this report.

A major cost factor in applying existing borehole techniques to a new application such as ER is the cost of calibrating each system for each specific combination of conditions that will be encountered. To understand the scale of the calibration problem, it is helpful to draw a comparison with the calibration of laboratory analytical instrumentation. To calibrate laboratory gamma-ray spectrometers, for instance, a number of standards must be prepared containing accurately known constituents in the same geometry as the unknown samples that are to be analyzed, and any deviation of the samples from the standards (for instance, different density) must be understood and corrections applied.

Precisely the same calibration requirements hold true for borehole spectral gamma-ray instrumentation except, instead of small cans or bottles of material, standards that simulate the borehole environment are needed. In the case of gamma-ray spectrometry, that typically means a model at least one meter in diameter by two or three meters high with a borehole of the appropriate diameter down the center. The model must be homogeneous or contain a known distribution of radioactive material. The model must be carefully analyzed and characterized, with all physical and chemical properties that affect gamma-ray attenuation understood. Ideally, a number of such models representative of the range of environments expected to be encountered in actual boreholes are needed, possibly including different borehole diameters, casing and borehole fluid, formation porosity and saturation, and all other factors which affect gamma-ray attenuation and absorption. The models should be traceable back to a recognized standard (regulatory agencies will require this if the data are to be used in planning and decision making). Any deviation of the actual borehole environment from the models must be understood and corrections applied as required[37,38]. The process of determining such correction factors is generally more difficult than in the case of laboratory instruments because of the difference in scale.

Physical models may take the form of test columns or test boxes composed of doped concrete, quarried rock, or other material designed to simulate the borehole environment as needed to meet the calibration requirements of a particular logging system. Many physical calibration models of that type already exist, including a number in the DOE complex and at other government facilities. For instance, doped concrete models were used extensively in the NURE Program in the U.S.{39} and in similar programs in other countries{40}, as well as in the petroleum industry{41,42}. Quarried rock models have been established at the U.S. Geological Survey in Denver{43}, at the Nevada Test Site{44}, in the petroleum industry and elsewhere. In some cases, models are made of loose material encased in a shell of aluminum, plastic or other material; if necessary, suitable experiments or computer modeling can be used to account for the effect of the shell. This approach has been used at the Nevada Test Site{45} and elsewhere.

Due to cost and other constraints, the number of physical models available for calibration is usually not sufficient to cover all conditions encountered in the field. Frequently, computer simulations are used to supply additional information. Experimental data from physical models can be used to benchmark computer simulation programs for parameters that are easy to model physically. Other parameters that are difficult or impossible to model physically can then be studied using the computer simulations. For instance, it is a relatively straightforward task to evaluate the response of a given logging system in a totally dry physical model and in a second model totally saturated with water. Achieving known, intermediate values of saturation using physical models can be difficult or impossible. Computer simulation programs, once benchmarked at 0% and 100% saturation, can extend the calibration results to intermediate values. Such simulations can also extend the calibration to include such factors as trace elements, different formation densities, and many other real-world conditions that may need to be studied and included in the calibration, data reduction and interpretation.

Even with extensive use of computer simulations to assist in the calibrations, building high-quality physical calibration models is costly. Costs can be minimized by designing and building the models to serve multiple users, following the examples of the American Petroleum Institute borehole calibration facilities in Houston and the DOE NURE calibration facilities in Grand Junction. This approach is particularly reasonable for the DOE complex, where all models are funded by the same agency. Another way to reduce costs might be to arrange for the high quality, underutilized and inexpensive Russian research institutes to participate in building and characterizing the models, an approach that offers potential geopolitical gains as well.

D. Thin bed effects

A properly calibrated nuclear borehole logging instrument can give accurate results in thick zones or regions where rock properties vary slowly, if appropriate correction factors are applied for non-standard borehole conditions. However, the logs will still be distorted in the vicinity of bed boundaries; thin zones (less than a meter or so), in particular, give rise to data that can be very inaccurate. To correct for such distortion, additive and multiplicative correction factors are not sufficient. Inverse theory must be applied to correct for the "smearing" effect of the spatial response of the logging instrument; this is sometimes called spatial deconvolution. In the case of passive SGR logging, this smearing effect is due largely to the fact that rock is translucent to gamma rays; the effect is a non-linear function of a number of borehole and formation parameters including borehole diameter, casing type and thickness, and borehole fluid, as well as formation density, porosity and water saturation, and other factors that affect the passage of gamma radiation through matter{46-52}.

Spatial deconvolution techniques, which have proven superior to detector collimation and other approaches, were used to detect substantial errors in the published radionuclide concentrations of a thin-zone gamma-ray logging test and calibration facility at DOE's Grand Junction installation during the NURE program{53}. Those errors, which had gone undetected throughout twenty years of logging instrument tests and calibrations in that model, were confirmed by subsequent physical sampling and laboratory analysis. The application of linear inverse theory to nuclear borehole data is not valid for all geologic/borehole environments. More sophisticated approaches may be needed for some environmental applications to meet the more stringent quality assurance requirements of the data quality objectives in ER work. In addition to passive SGR logging, these processing techniques may be extended to other borehole logging methods as well{54-57}.

IV. RADIATION TRANSPORT SIMULATIONS: AN OVERVIEW

To understand the behavior of a complicated instrument such as a neutron-induced gamma-ray spectroscopy system requires a great deal of detailed study. There are several methods available for carrying out such studies. The instrument can be run in a variety of boreholes that have been extensively studied by other means, such as laboratory analysis of core samples. While attractive at first glance, this approach suffers from the fact that we rarely know in the required degree of detail exactly what the complex physical and chemical properties of the subsurface are in the vicinity of the borehole. In addition to spatial inhomogeneities inherent in the undisturbed rock, the drilling process alters the formation properties and, in general, the nature and extent of these changes are not known with certainty. For these reasons, we consider tests in boreholes to be primarily useful in the later stages of development to confirm instrument behavior that has been ascertained by better-controlled techniques. Theoretical calculations can be useful for developing a general understanding of some aspects of system behavior but cannot begin to handle the complexity of an real-world instrument in an actual borehole environment. Thus, the two techniques of choice for the earlier stages of development are physical modeling and computer simulations.

Physical models tend to be costly, especially with the strict safety and environmental regulations that exist today. Furthermore, if the behavior of the instrument is to be ascertained for typical field applications, there are many factors that must be studied over a range of borehole and formation conditions, such as borehole diameter, casing, rock chemistry and density, instrument geometry, and contaminants. Some of these factors interact, and the number of model borehole configurations that would be needed to sort out the various combinations of conditions would be dozens at a minimum. In addition, we do not have the kind of detailed and precise control over the properties of physical models that would be required to explore all of the factors that could be affecting the data. Thus, while this approach provides important basic understanding of instrument behavior it is not suitable for sorting out the details.

Computer codes that simulate nuclear processes are widely used in nuclear engineering applications such as radiation shielding design and criticality studies. Computer simulations have also been used by a number of organizations around the world to help design and understand many nuclear processes, including the behavior of nuclear borehole logging instruments. The theory behind radiation transport simulations is well understood, as is the process of applying the theory numerically. The accuracy of the results is limited mainly by the accuracy of the nuclear data libraries used by the software.

We concluded that a combination of all of the above approaches would be the most cost-effective and reliable in characterizing borehole instruments. A few well-understood physical models are required to achieve a basic calibration of the instrument. Computer codes are benchmarked and validated using the experimental data from the physical models. When an acceptable agreement is achieved between experimental and simulated data for several sets of conditions, computer simulations are used to study numerous sets of conditions, including a variety of instrument designs, all of which would be difficult or prohibitively expensive to do using any other approach. Finally, the instrument will be tested in well-characterized field boreholes as a final confirmation that everything is working as anticipated.

A. Choosing a computer simulation approach

There are two main computational approaches to the computer simulation of radiation transport processes, (a) statistical and (b) deterministic. These approaches have advantages and disadvantages that make them more or less useful depending on the nature of the problems being studied and the goals of the modeling effort.

1. Monte Carlo codes

   The statistical simulation codes commonly used in nuclear transport simulations are called "Monte Carlo" because their execution is guided by repeated throws of computerized dice, i.e., a numerical random number generator. These random numbers are used, along with probability functions representing each of the categories of events that can occur, to determine what happens. For example, in a simple Monte Carlo simulation with a known distribution of gamma emitting nuclides and a gamma-ray detector, a random number is used to select the coordinates of the nuclide that will emit the next gamma ray to be followed, based on the half-life of that isotope relative to other isotopes that may be present and the concentration distributions of those isotopes. If the gamma-ray energy spectrum of the emitting isotope is not monoenergetic, another random number is used to determine the energy of the gamma ray based on the known emission spectrum. The initial direction of the emitted gamma ray is a uniformly distributed random function and is determined by another random number. This process continues, using random numbers and appropriate probability functions to determine the point of the first interaction of the gamma ray with matter in the vicinity, the type of interaction, what radiation is given off following that interaction, and so forth. If a gamma ray reaches the detector, the process of detection can be simulated in an analogous manner.

   This simple approach can produce accurate results if properly performed. However, it can also be extremely inefficient depending on the geometry being simulated. This is the case with neutron-induced spectral gamma-ray borehole logging. To simulate gamma rays emitted following the capture of a thermal neutron by a nucleus using the straightforward approach described above, each neutron must be tracked from its emission at an energy of 14.1 MeV through numerous interactions down to thermal energy (nominally 0.25 eV), captured, a gamma ray given off, and that gamma ray tracked as it makes its way through the medium. This represents dozens of calculations per neutron. Of course, the vast majority of gamma rays never reach the detector. On the order of 10^5 neutrons are emitted for each gamma ray detected. Finally, a typical high energy-resolution gamma-ray spectrum with good statistical accuracy could represent some 10^7 detected gamma rays. Based on these figures we can see that roughly 10^{14} calculations (not 10^{14} particles -- each particle requires many calculations) are required to produce one good gamma-ray spectrum.

The huge overhead in computation time described above is the chief drawback of Monte Carlo codes. To make the technique more efficient, a variety of modifications have been introduced over the years. For example, a number of sophisticated variance reduction techniques have been devised to reduce the number of pointless calculations that can occur. For instance, when a neutron wanders so far away from the detector that it is very unlikely that any emitted gamma ray could be detected, it is no longer tracked. Also, techniques such as correlated sampling can be used to simulate the effects of small changes in the physical conditions, such as substituting one trace contaminant for another.

2. Deterministic models

   The deterministic or non-statistical computer simulation approach commonly used for simulating nuclear logging devices is multigroup diffusion, which includes such techniques as discrete ordinates methods. Multigroup diffusion codes make a number of simplifying assumptions about the geometry, material properties and energy distributions of the particles to make the problem tractable. This greatly reduces computation time compared with Monte Carlo techniques and can be very useful in certain limited applications. Such techniques could have played a limited role in this project, but since they are not general enough to handle the complexity we are dealing with, and since we have limited resources to devote to addressing the computer simulations, we chose to pursue the more generalized simulation approach, Monte Carlo.

B. Choosing a Monte Carlo code

The principal criteria for evaluating the Monte Carlo simulation software are, in arbitrary order: cost, accuracy (including quality assurance issues), speed for production calculations, foreign vs. domestic procurement, and availability of support. Several publicly-distributed families of Monte Carlo computer simulation programs are commonly used for simulating nuclear borehole logging instrumentation. These include two U.S.-based programs as well as programs produced and maintained in other countries.

MCNP[58] is maintained and distributed by Los Alamos National Laboratory and, at the current time, is readily available at no cost. MCNP is primarily intended for radiation shielding and criticality calculations and it is the state of the art code for those applications. A great deal of money and effort have been expended in developing, testing and improving the program. However, we have found it to be somewhat intractable for our particular application because it has not been optimized for simulating neutron-induced gamma-ray spectroscopy problems.

Codes such as McDNL, McPNL, and McLLS have been developed at North Carolina State University by the Nuclear Engineering Department{61-64}. They are available at moderate cost but are supported at a low level relative to MCNP. The design of these programs offers some advantages over MCNP for this application, so we are testing these programs as well.

McBEND{65-67} is maintained at the Harwell research establishment in Great Britain and serves a similar function to MCNP, including the simulation of nuclear borehole logging devices. McBEND has a perturbation option, DUCKPOND, that allows the effects of small changes in the environment to be estimated without the overhead of running a full-blown calculation each time. While McBEND would probably be suitable for modeling this problem, the possible difficulties in international distribution and support stopped us from seriously considering that simulation package for this project. Programs from other countries{e.g. 68-72} were rejected for this same reason.

C. Obtaining experimental data

At the time that we received funding for this project, our plan as set forth in the TTPs was for RUST Geotech (DOE/GJPO) and the U.S. Geological Survey to put together a test system capable of gathering data that could be used to evaluate and benchmark the computer simulation codes. At about the same time, we became aware that there was a newly formed small company that had the capability to make the experimental measurements. In keeping with DOE's emphasis on commercialization and cooperation with industry, Geotech modified their work plan and schedule, in consultation with DOE, to include commercial participation. This substantially delayed the experiments to be performed under TTP No. AL931001. Since the computer simulations for which Los Alamos has responsibility need experimental data for benchmarking, the simulations were also delayed somewhat. We (Los Alamos) approached Schlumberger Well Services and Environmental Measurements Corporation (EMC) to see if either would be willing to supply data that we could use to benchmark our computer simulations in the absence of the data from DOE/GJPO. We eventually received two spectra from EMC, so we chose to simulate their instrumentation. Thus, by June, 1993, we were in possession of data that allowed us to begin limited benchmarking of the computer programs.

V. THE MCNP SIMULATIONS

MCNP has impressive credentials and is recognized world-wide as an important program for general nuclear transport simulations. Furthermore, it is widely used in the petroleum industry to simulate nuclear borehole logging systems.

We have found that MCNP in its present form is only marginally suitable for simulating neutron-induced gamma-ray spectroscopy problems. At best, it requires a number of compromises and workarounds. For instance, correlated sampling, a technique for testing the sensitivity of the simulated system to small changes in the environment, could be very useful for this application, but is only available as a patch for an earlier version of MCNP; that version is currently unsupported and lacks some of the features of the currently supported version. Correlated sampling is scheduled for inclusion in the next release of MCNP, but that release will likely be too late to be useful for this project. Other limitations of MCNP for this application will be discussed below.

A. Geometry and material assumptions

The experimental data used for benchmarking MCNP in FY-93 were measured in the Atlas Wireline Services glass plate model. This model consists of 1.27 cm thick glass plates stacked with 0.42 cm spacers. The model includes a borehole of 15.7 cm ID encased by 2.1 cm thick steel-casing and a 2.86 cm thick layer of cement as shown in Figure 5.1. The borehole was filled with a sodium bromide solution, 1.19 g/cm^3 of powdered NaBr added to tap water titrated at 103 ppm NaCl by weight. Data were obtained with the voids between the glass plates (but not the borehole) filled with two different saline solutions during two separate experimental runs. The concentrations of the solutions were 3099 ppm and 10418 ppm NaCl. No passive SGR measurements were available for correcting the data for background radiation.

Schematics of the nuclear well-logging instrument package (or "tool" as the borehole sonde is called in the petroleum industry) were provided by EMC and as much detail as possible was included in the MCNP geometry specification for this tool. The tool uses a 14-MeV pulsed neutron generator as the neutron source and a high-purity germanium (HPGe) detector. The generator nominally operates at 1 - 3 kHz and is located below the detector. The MCNP representation of the tool is shown in Figure 5.2. In the benchmark simulation, the tool shown in Figure 5.2 was represented as eccentered (placed against the borehole wall) in the borehole shown in Figure 5.1.

The MCNP material specifications for the glass-plate model and the tool are listed in Tables 5.1 and 5.2, respectively. Dr. Gary Meyers of EMC stated that the unit ppm denoted the concentration by number instead of the usual

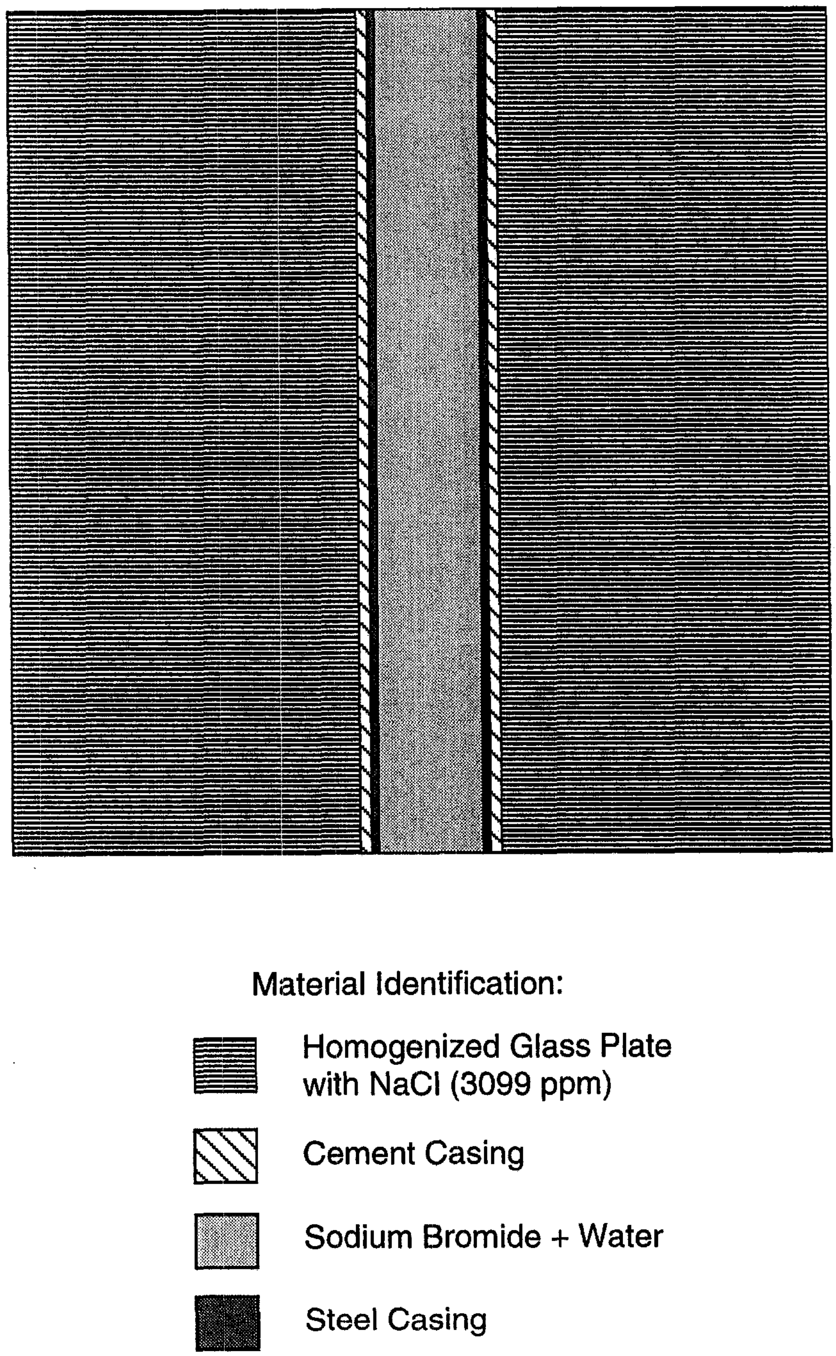

Figure 5.1: *Geometry and materials used to simulate the glass plate model.*

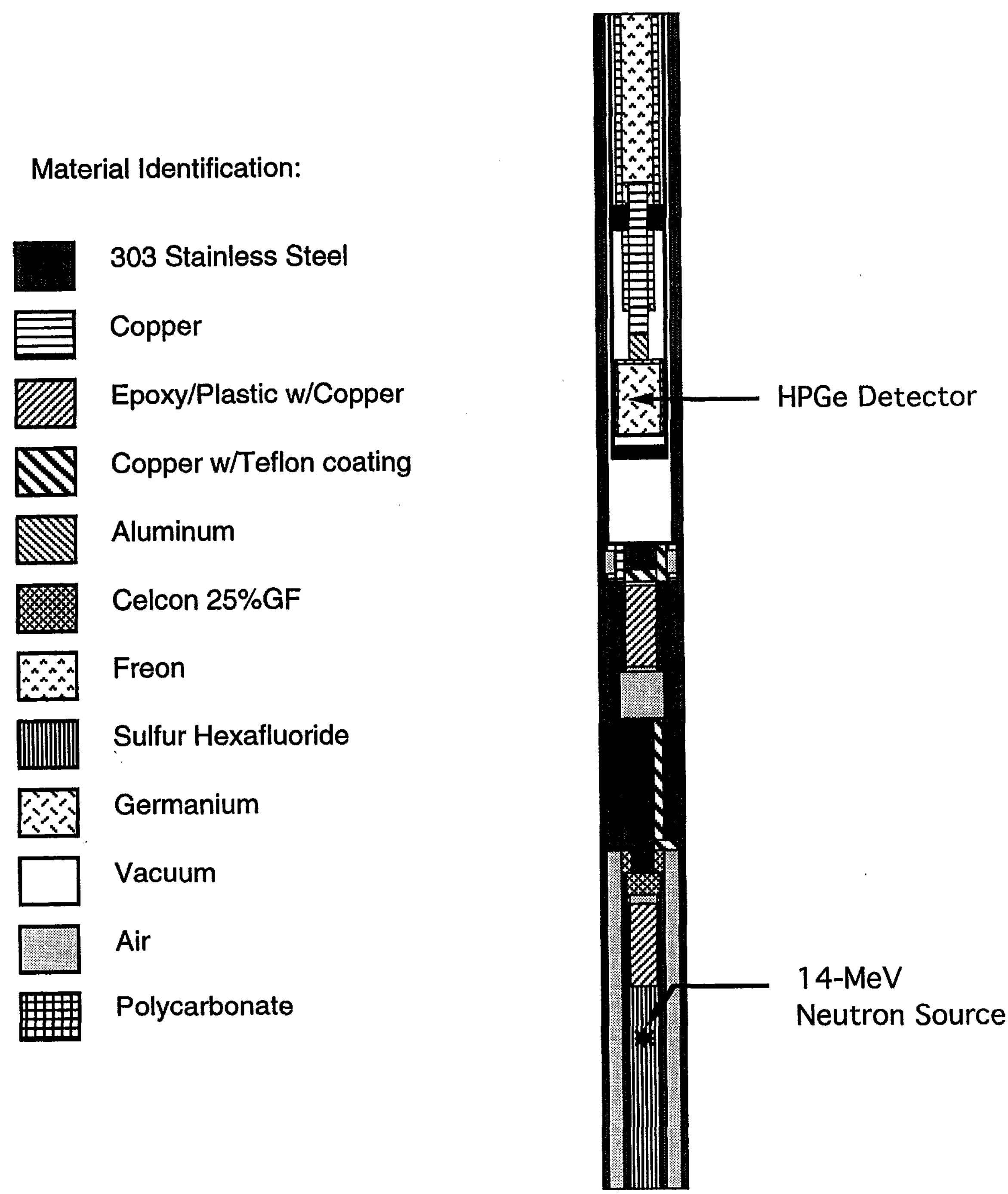

Figure 5.2: *Geometry and materials used to simulate the EMC capture tool.*

concentration by weight. This resulted in the MCNP simulation using 9984 ppm by weight (0.9984% by weight) of NaCl instead of 3099 ppm (0.31% by weight). Therefore, the amplitude of the Na and Cl gamma-ray lines in the MCNP simulation would be reduced by a factor of approximately 3.23 if a specification of 3099 ppm by weight were used rather than 3099 PPM by number. The two experiments with two different NaCl concentrations were performed to ascertain the capability of this tool for detecting Chlorine. Since there was no appreciable difference in the experimental data for the two salinities as shown in Figure 5.3, only the 3099 ppm problem was simulated using MCNP.

B. Time gating

The EMC instrument uses two time gates for accumulating two gamma-ray spectra. One gate corresponds to the period during which the neutron generator is producing a burst of neutrons. The associated spectrum is loosely referred to as the inelastic spectrum. Another gate corresponds to the period between the neutron bursts. The associated spectrum is referred to as the capture spectrum. It is the capture spectrum that will be most useful in Multi-Spectral logging for determining the concentrations of various nuclides of interest in the formation.

C. Variance reduction

The MCNP simulation used some standard variance reduction techniques to obtain better statistics at the detector location{73-76}. The source was directionally biased such that a half-cone of angle 45° was not sampled in the direction opposite the ray from the neutron source to detector. The variance reduction techniques of using weight-windows in space and energy were also used. There were six energy bins (ranges) used for both neutrons and photons. The neutron energy bins were 1×10^{-5}, 1×10^{-3}, 1×10^{-2}, 1.0, 10.0, and 15.0 MeV where the bin is specified by the upper energy limit. The photon energy bins were 2.0, 4.0, 6.0, 8.0, 10.0, and 24.0 MeV. A large upper-energy bin for the photons was used since the EMC data were sparse above 7.5 MeV.

Figure 5.3: EMC Glass-plate Model Data from 0.0-8.0 MeV.

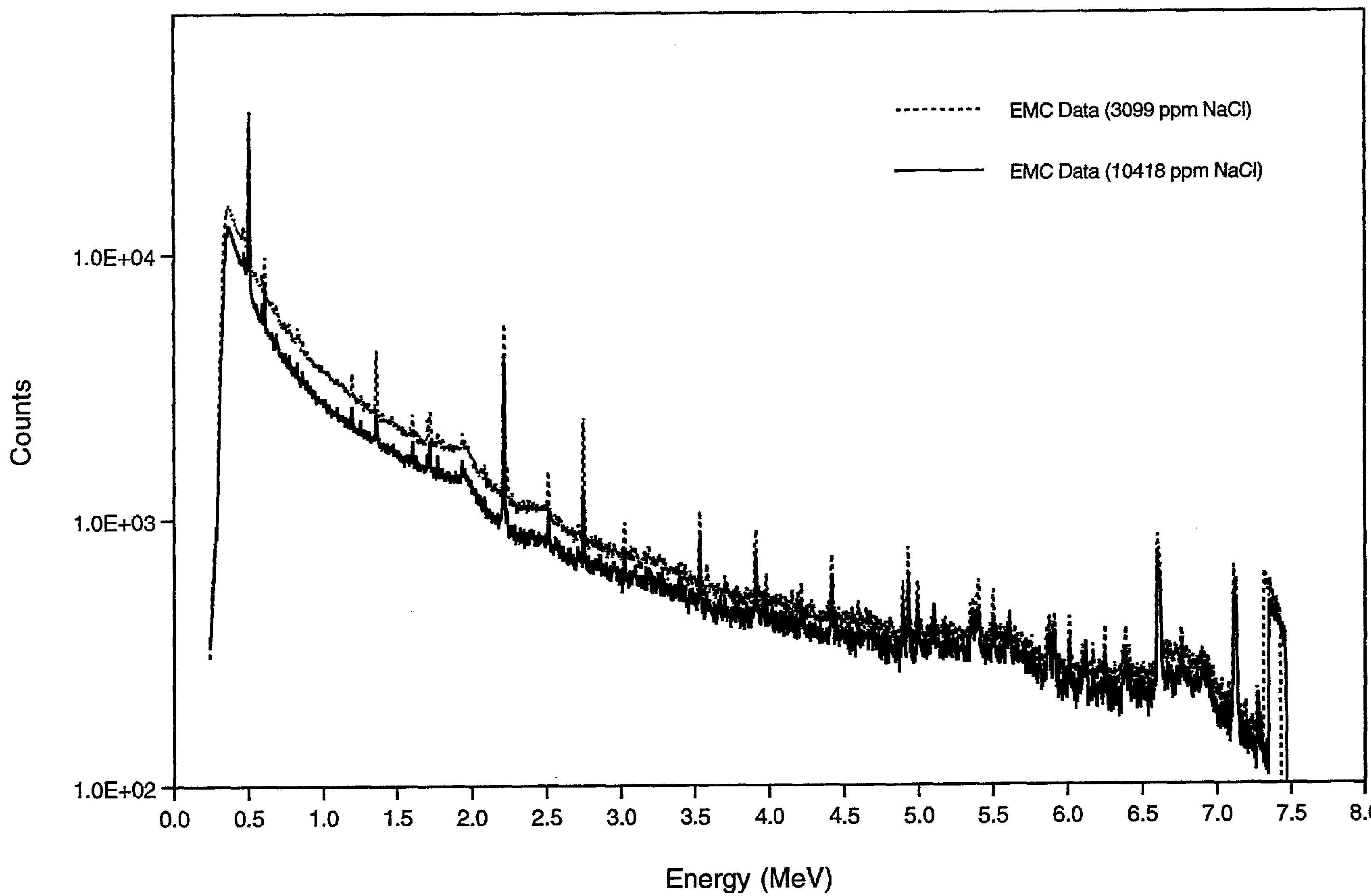

Table 5.1

MCNP Material Specification for the Glass-plate Model

Material Description	Density grams/cc	Z (Atomic #)	Element or Isotope	Weight Fraction
Sodium Bromide plus tap water titrated at 103 ppm NaCl.	1.189	1	H	0.09411
		8	O	0.747
		11	Na	0.03572
		17	Cl	1.70E-04
		33	Br	0.123
Steel-casing, L-80/API 5AC.	7.934	6	C	0.004
		14	Si	0.0035
		15	P	0.0004
		25	Mn	0.019
		26	Fe	0.9671
		28	Ni	0.0025
		29	Cu	0.0035
Portland Type H Cement.	1.92	1	H	0.0369
		8	O	0.5376
Heavy Cement: 33% H_2O + 67% Cement mix at 3.10 g/cc		12	Mg	0.0066
		13	Al	0.0352
		14	Si	0.0638
		16	S	0.007
		26	Fe	0.0352
		20	Ca	0.2777
Homogenized Glass Plates and tap water titrated to 3099 ppm NaCl.	2.238	1	H	0.01245
		5	10B	3.54E-06
		5	11B	1.43E-05
Glass: 99.98% SiO2 + 0.002% B		8	O	0.5716
Salt water: 99% H_2O + 1% NaCl		11	Na	4.43E-04
Combination: 88.75% glass + 11.25% salt water		14	Si	0.4148
		17	Cl	6.89E-04

Table 5.2

MCNP Material Specification for the EMC Capture Tool

Material Description	Density grams/cc	Z (Atomic #)	Element or Isotope	Weight Fraction
303 Stainless Steel	7.95	6	C	0.0015
		14	Si	0.01
(also used in place of		15	P	0.002
17-4 Ph Stainless Steel)		16	S	1.50E-04
		24	Cr	0.18
		25	Mn	0.02
		26	Fe	0.69635
		28	Ni	0.09
Freon-12	1.52	6	C	0.0993
		9	F	0.5865
		17	Cl	0.3142
Aluminum	2.7	13	Al	1.0
Germanium (no MCNP cross-sections available)	5.32	32	Ge	1.0
Copper	8.96	29	Cu	1.0
Polycarbonate	1.4	1	H	0.1
		6	C	0.61
		8	O	0.29
Celcon, 25% GF	1.62	1	H	0.0495
		6	C	0.3038
		8	O	0.5299
		14	Si	0.1168
Sulfur Hexaflouride	0.0412	9	F	0.7805
assumed 100 psi		16	S	0.2195
Air	0.00129	7	N	0.765
sea level (0.00129 g/cc)		8	O	0.235
Los Alamos (0.000935)				
Connector plus Copper wire.	5.53	1	H	0.0726
Assumed polycarbonate for connector.		6	C	0.4427
		8	O	0.2104
		29	Cu	0.2743
Copper wire with teflon coating	various	6	C	0.179
		9	F	0.5677
		29	Cu	0.2533

D. Results of simulations

The first simulation was run on an HP-730 workstation (32 Mbytes of RAM) for 6460 minutes of CPU time, tracking 7.078×10^6 source neutrons. A second simulation was run after the workstation had been upgraded to an HP-735, giving it a faster CPU and 112 Mbytes of RAM. This second simulation used 14,500 minutes of CPU time, tracking 3.596×10^7 source neutrons. The improvement in computing power resulted in an increase in speed of a factor of 2.19 for the MCNP code; for roughly twice the computer time, the number of source neutrons tracked was increased by a factor of four.

The results for the MCNP simulation and from the experimental data are listed in Table 6.3. The capture spectrum for the MCNP simulation and the corresponding EMC data are shown in Figures 5.4 and 5.5 respectively. All capture gamma-ray lines observed experimentally are reproduced by MCNP. In addition, the MCNP simulation shows nine distinct Cl lines (1.165, 1.959, 4.980 5.715, 6.111, 6.620, 6.978, 7.414, and 7.790 MeV) over the energy range from E_γ=0-8 MeV. There is no evidence for these Cl lines in the EMC data for either salinity.

E. Limitations of the code

The simulation of the EMC glass-plate experiment indicates that MCNP can simulate experimental results with several important constraints. For this application, MCNP is primarily limited by the availability and quality of the neutron cross-sections. In particular, some photon production cross-sections have wide energy bins (50 keV in the case of iron) representing the gamma-ray lines from neutron capture. This has the tendency to obscure capture gamma-ray lines from other nuclides that may be present in that energy range. For example, the Cl lines at 1.165 MeV and 6.111 MeV have roughly the same intensity but the lower energy line is obscured by the wide Fe bin as shown in Figure 5.6. There is the possibility of making a minor modification of the code to allow the user to request the spectra produced by each element or isotope of interest, as well as the total spectrum. We are pursuing this option with Los Alamos group X-6.

The unavailability of Ge cross-sections for use with MCNP makes the actual detector response difficult to simulate. The efficiency of the detector cannot be reproduced, there is no generation of escape peaks, and MCNP is unable to simulate the gamma rays from Ge(n,γ) reactions seen experimentally below about 1.5 MeV. The MCNP detector response is the response that would be obtained by a 'perfect' detector, accurately detecting all gamma rays entering its space and generating no escape peaks. Los Alamos group

Figure 5.4: MCNP Simulation of the EMC Glass-plate
Model (3099 ppm NaCl) from 0.0-8.0 MeV.

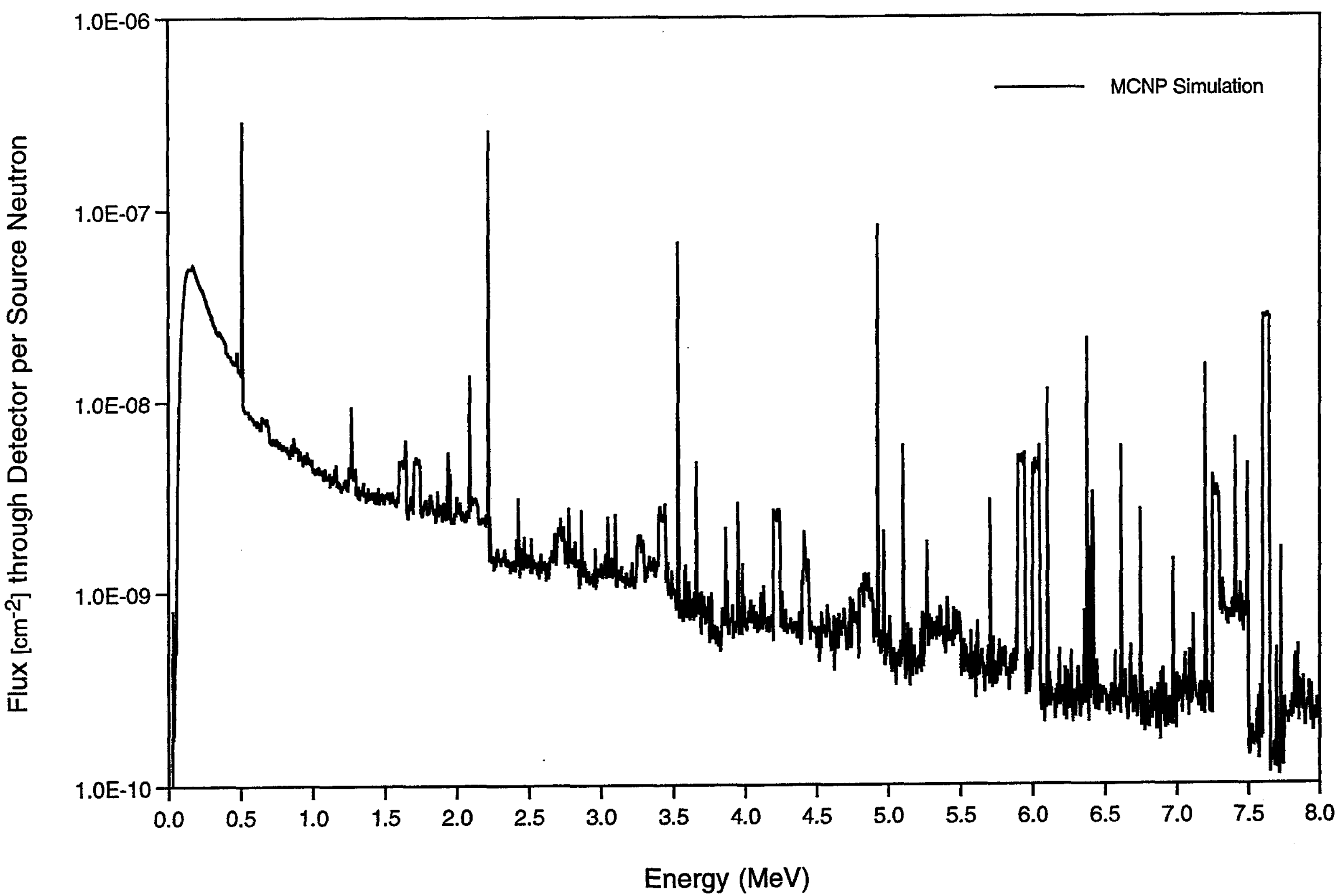

Figure 5.5: EMC Glass-plate Model Data
(3099 ppm NaCl) from 0.0-8.0 MeV.

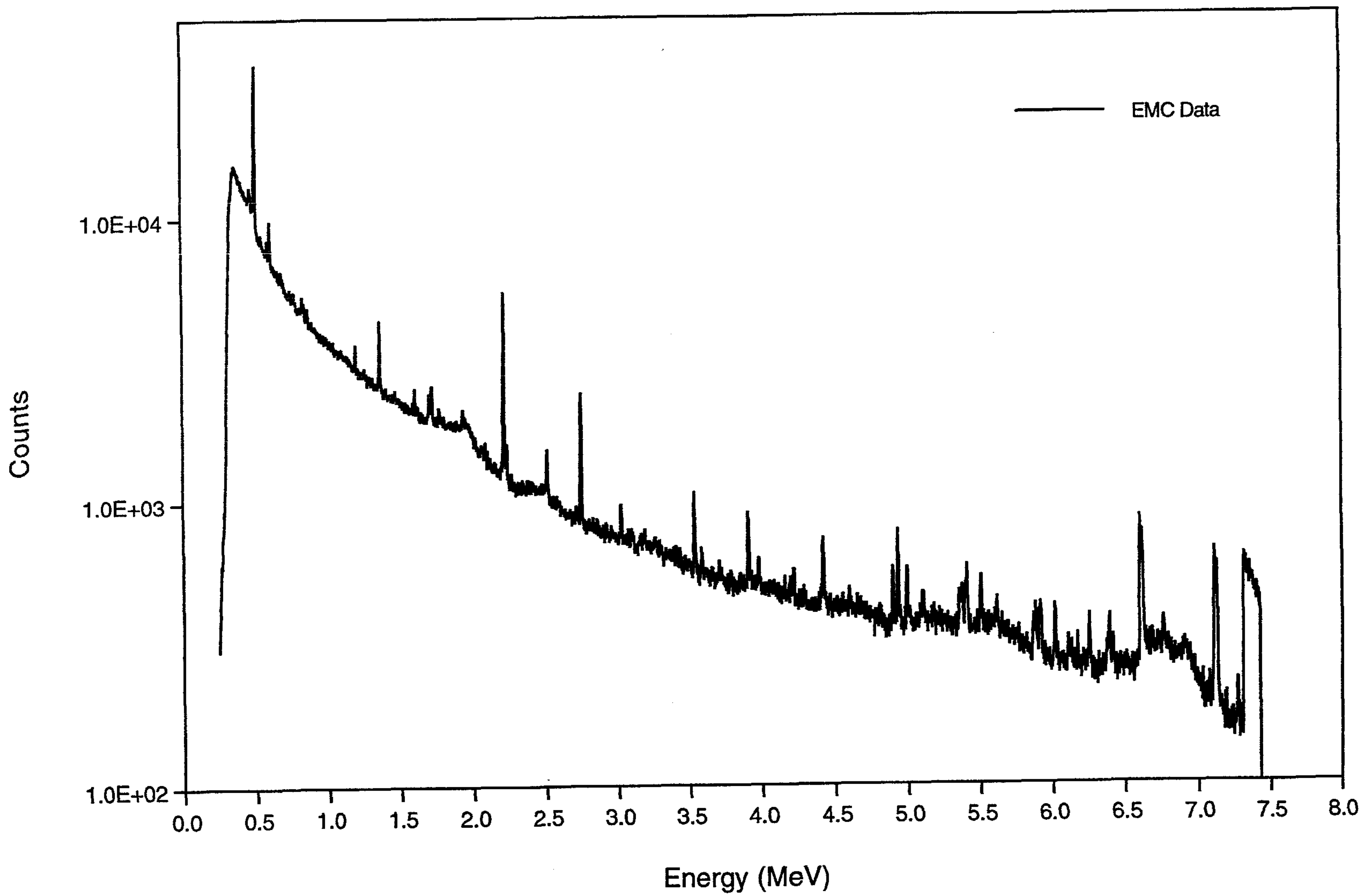

Table 5.3

Identification of Capture Gamma-Ray Lines

Listed below are the gamma rays identified in the MCNP simulation and the EMC experimental data over the energy range from 0.0 to 8.0 MeV. The gamma-ray energies highlighted by **bold type** are those peaks observed in the experimental data from EMC, while the observed gamma rays from MCNP are indicated in the right-hand column.

MCNP Peak Energy (MeV)	Actual Peak Gamma-ray Energy (MeV)	Single Escape Peak Energy (MeV)	Double Escape Peak Energy (MeV)	Gamma-ray Peak Identification
0.375	0.352, 0.367			Fe
0.472	**0.474, 0.479**			Na, Fe
0.5125	**0.511**			pair prod.
	0.555			Br (?)
	0.596			Ge
	0.619			Br (?)
	0.664			
0.692	**0.692**			Fe
	0.748			Cr
	0.777			K
	0.831			Cr
	0.844			
	0.868			Ge
	1.019			Fe
	1.043			Br (?)
	1.199			Br (?)
1.2725	1.273	0.762	0.251	Si
	1.366	0.855	0.344	
1.625	**1.613**	1.102	0.591	Fe
1.6475	1.165	0.654	0.143	Cl
	1.708	1.197	0.686	
1.725	**1.725**	1.214	0.703	Fe
	1.775	1.264	0.753	Al
1.942	**1.942**	1.431	0.920	Ca
1.9575	1.959, 1.951			Cl
2.0925	2.093	1.582	1.071	Si
2.2225	**2.223**	1.712	1.201	H
2.2325	2.233-2.241			K, Si, Cr, Al
2.4125	2.415	1.904	1.393	Na
2.4275	**2.426**	1.915	1.404	Si
2.730	2.721	2.210	1.699	Fe
2.7825	**2.782**	2.271	1.760	Si
2.8675	2.863, 2.864			Na, Cl

Table 5.3 (cont'd)

Identification of Capture Gamma-Ray Lines

MCNP Peak Energy (MeV)	Actual Peak Gamma-ray Energy (MeV)	Single Escape Peak Energy (MeV)	Double Escape Peak Energy (MeV)	Gamma-ray Peak Identification
2.9625	2.960	2.449	1.938	Al
3.0575	3.054, 3.061			Si, Cl
3.1025	3.102	2.592	2.081	Si
3.275		2.764	2.253	Fe
3.425	3.413, 3.436			Fe
3.5325	**3.539**	**3.028**	**2.517**	Si
3.5875	**3.588, 3.591**	3.077, 3.080	2.566, 2.569	Na, Al
3.610	3.610	3.099	2.588	Ca
3.6625	3.661	3.150	2.639	Si
3.8675	3.865	3.354	2.843	Si
3.8775	3.878	3.367	2.856	Na
3.9525	3.955	3.444	2.933	Si
3.9825	**3.982**	3.471	2.960	Na
4.225	**4.218**	3.707	3.196	Fe
4.4175	**4.419**	3.908	3.397	Ca
4.425	4.406	3.895	3.384	Fe
4.850	4.810	4.299	3.788	Fe
4.9325	**4.934**	**4.423**	**3.912**	Si
4.9725	4.980	4.469	3.958	Cl
5.1075	5.107	4.596	4.085	Si
5.2725	5.271	4.760	4.249	Ca
5.6175	**5.617**	**5.106**	**4.595**	Na
5.7075	5.715	5.204	4.693	Cl
5.925	**5.920**	**5.409**	**4.898**	Fe
6.025	**6.018**	**5.507**	**4.996**	Fe
6.0475				
6.1075	6.111	**5.600**	**5.089**	Cl
6.3625		5.852	5.341	
6.3825	**6.381**	**5.870**	**5.359**	Si
6.3975	**6.395**	**5.884**	**5.373**	Na
6.420	**6.420**	**5.909**	**5.398**	Ca
6.6175	6.620, 6.628			Cl
6.7475	6.743, 6.747	6.232, 6.236	5.721, 5.725	Si
6.9775	6.978	6.467	5.956	Cl
7.1125	7.100			Cr?
7.2025	7.201	6.690	6.179	Si
7.275	7.279	**6.768**	**6.257**	Fe
7.4125	7.414	6.903	6.392	Cl
7.4975		6.987	6.476	
7.625	7.631, 7.645	**7.120, 7.134**	**6.637, 6.623**	Fe
7.7275	**7.723**	7.212	6.701	Al
7.8475	7.790	7.279	6.768	Cl

X-6 is currently processing Ge cross-sections for us and these should be available early in 1994.

Some neutron cross-sections are unavailable due to lack of experimental data, while others are unavailable because existing data have not been processed into the MCNP format. The latter problem is more easily addressed. Unavailability of cross-sections for some environmental contaminants due to a lack of experimental data is a problem that may be difficult to address in the future because of the current cutbacks in our national nuclear experimental facilities.

We are pursuing several approaches to improving MCNP for this type of application. First, we are commissioning some minor modifications to the code. Second, we are having some important cross-sections that are available as experimental data converted into the proper MCNP format. Finally, we hope to improve the accuracy of the photon production spectra in MCNP. These steps should contribute significantly toward making the simulations more reliable and accurate.

F. Comments about the hardware

It is easy to see that the perfect detector response of MCNP enables the identification of more capture gamma-ray lines than the experimental data. Since the HPGe detector in the EMC tool was physically so small, the detector had a limited efficiency (less than 8% relative to a 3"x3" NaI detector) and the experimental data are therefore relatively difficult to analyze. The spectra are predominately populated by the double and single escape peaks as opposed to the primary energy peak for each gamma ray. This makes the identification of the appropriate nuclides, as well as determining the overall strength for a particular gamma-ray line, more difficult.

The above observations should not be construed as a criticism of the EMC tool, which was designed for use under demanding conditions in the petroleum industry. However, for most environmental applications many of the constraints encountered in the design of the EMC tool can be relaxed substantially, allowing us to more closely approach the ideal detector system shown in the MCNP simulations. Using a substantially larger detector, a neutron shield around the detector, state of the art electronics, and other changes, we can expect to optimize detection thresholds and greatly reduce measurement time.

VI. THE NCSU SIMULATION CODES

The simulation codes written and maintained at North Carolina State University offer built in correlated sampling{63,64}, aggressive built-in variance reduction, and a way of handling the gamma-ray energy spectrum that is different from MCNP. As of the end of FY-93 NCSU was working to benchmark their codes to simulate the same experimental data used to benchmark MCNP, but results and details of the simulations were not yet available.

VII. CONCLUSIONS

In the DOE Environmental Restoration Program, techniques that reduce site characterization and monitoring costs and maximize the information obtained from each borehole are needed because drilling boreholes in contaminated areas and analyzing samples are grossly expensive procedures. Nuclear borehole logging techniques have proven their value in other applications, giving a continuous record of chemical composition along the borehole and typically analyzing 10^3 to 10^4 times more material than physical sample analyses.

In some cases, such as the carbonate logging at the Nevada Test Site described earlier, supplementing a reduced sample analysis program with borehole logging can reduce overall costs while enhancing data confidence. A reasonable goal in environmental work is to replace analysis of some borehole samples with nuclear borehole logging. Depending on our level of success in achieving that goal, we could save millions of dollars at each DOE site where these techniques are applicable.

In the case of long-term monitoring for gamma-emitting contaminants and quite possibly other contaminants as well, there is no reasonable substitute for in-situ SGR measurements combined with sophisticated data processing. This approach gives us a monitoring tool that is far superior to all other foreseeable technologies, with continuous coverage, large sample volume, sensitivity and accuracy, combined with the ability to run repeat measurements in the same borehole year after year at reasonable cost.

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APPENDIX A: BUDGET AND SCHEDULE

This project is a cooperative effort under three separate but related TTPs: TTP No. 131004 from Los Alamos National Laboratory, which includes effort by Lawrence Livermore National Laboratory, TTP No. AL931001 from DOE/GJPO produced by RUST Geotech, a DOE contractor, and TTP No. AL031001 produced by the U. S. Geological Survey. This Annual Summary Report is for TTP No. 131004.

A. Responsibilities

The technical approach for this joint project is divided into three categories: (1) computer simulations and interpretation theory, (2) hardware development, and (3) experiments and field work. The responsibilities for these three categories of technical effort are as follows:

1. Computer simulations and interpretation theory

   Los Alamos has the primary responsibility for the computer simulations and interpretation theory effort, with substantial support provided by GJPO and the USGS. That work is described in this report.

2. Hardware development

   DOE/GJPO (RUST Geotech) and the U. S. Geological Survey, working under TTP No. AL931001 and AL031001, respectively, share responsibility for the hardware development associated with this joint project. Our (Los Alamos) responsibility under TTP No. AL131004 is to provide technical support to DOE/GJPO for development of a new experimental prototype pulsed neutron induced gamma-ray spectroscopy logging system. This support will consist largely of participation in discussions and decisions regarding performance and design specifications based primarily on the information gained from the computer simulations, and continuing technical feedback throughout the hardware development process.

3. Experiments and field work

   DOE/GJPO (RUST Geotech), working under TTP No. AL931001, has primary responsibility for the hardware development. Our (Los Alamos) responsibility under TTP No. AL131004 is to provide advice and feedback to GJPO in support of the experiments and field work, which will consist of experiments in physical models to benchmark the computer simulations and obtain separate estimates of detection thresholds for a few nuclides of interest along with possible tests in selected field boreholes at DOE waste sites. We will cooperate with DOE/GJPO participants in designing suitable experiments and field tests. We will participate in data analysis and interpretation, based on the simulations and interpretation theory.

B. The original proposal

The original proposal consisted of a single TTP submitted by Los Alamos in collaboration with DOE/GJPO (RUST Geotech) proposing a joint effort that included DOE/GJPO Geotech and Highland Scientific, a technical consulting firm owned and operated by Robert Wilson who subsequently joined the staff of Geotech. Phase I of this project was budgeted for $260k to perform a feasibility study based on experiments and computer simulations along with the minimum hardware modifications required for running the proof of principle experiments. A decision point during FY-93 would evaluate whether the technology appeared to be useful for ER; if so, Phase II would involve development of an experimental prototype for testing, evaluation and demonstration. No field-ruggedized equipment would have been built under the original proposal. The original proposed budget is shown in Table A.1.

Table A.1 (Dollars in Thousands)

	FY-93	FY-94	FY-95	TOTAL
RUST Geotech	$204	$216	$0	$420
Los Alamos	$142	$147	$0	$289
Total	$346	$363	$0	$709

C. The proposal as funded

The CMST-IP directed Los Alamos and RUST Geotech to work with Oak Ridge and the USGS, organizations that had submitted vaguely related proposals, to come up with a combined proposal. At the same time, a second Los Alamos proposal submitted by John Conaway, "Quantitative Spectral Logging," was thrown into the mix. We were directed to produce a proposal wherein the feasibility study and the development of the experimental prototype would be done in parallel, and we were told to extend the project to include building and testing a production prototype system.

We had a meeting which included PIs from Los Alamos, RUST Geotech, the USGS and Oak Ridge, along with Bill Haas representing the CMST-IP. Oak Ridge subsequently dropped out, stating that they had ascertained that there was little requirement for their proposed technology. Eventually a joint proposal involving Los Alamos, RUST Geotech and the USGS evolved. (The second Los Alamos proposal (Quantitative Spectral Logging) was left as a separate proposal and in the end was not funded in FY-93; it was later funded for FY-94 and combined with the Los Alamos portion of the Multi-Spectral project).

The joint proposal was approved and the participants were directed to submit separate TTPs for the RUST Geotech and USGS efforts in addition to the Los Alamos TTP. Los Alamos received funding in late January, 1993. The USGS did not receive their FY-93 funding until the final weeks of FY-93. The budget as approved for funding in FY-93 is shown in Table A.2.

Table A.2 (Dollars in Thousands)

	FY-93	FY-94	FY-95	TOTAL
RUST Geotech	$245	$323	$0	$568
USGS	$95	$239	$0	$334
Los Alamos	$205	$287	$0	$492
Total	$545	$849	$0	$1,394

D. Changes following funding in FY-93

Early in the project (January, 1993) the participants identified a small, newly formed company, Environmental Measurements Corp. (EMC), that has the capability of doing some of the experimental work called for in the TTPs. A second company, Schlumberger, also has done significant work in this area of technology. Recognizing that collaboration between national labs and industry is a high priority with DOE and the federal government, the participants consulted with a number of people inside our organizations, at Ames National Lab, and in DOE, about collaborating with an industry partner Responses were consistently affirmative. Since the experimental work was covered by the DOE/GJPO TTP, RUST Geotech began the process of obtaining formal approval for this change.

E. Changes for FY-94

The original purpose of this project was to evaluate neutron-induced spectral gamma-ray borehole logging for mapping contaminants *in situ,* and that effort continues. In addition to this continuing joint project, a new project has been folded in beginning in FY-94 based on another TTP, No. AL141005. This second project is to be performed primarily by Los Alamos with Westinghouse Hanford Corporation participating under their own ER funding. The goal of this second project is to put passive spectral gamma-ray (SGR) borehole logging on a firm quantitative basis so the data are acceptable to regulatory agencies in the same way that laboratory analyses of core samples are now acceptable. This effort is needed because SGR borehole logging is capable of identifying gamma-emitting contaminants such as ^{137}Cs *in-situ*, but the data are generally not proportional to the concentrations of contaminants at a given depth.

F. Administrative problems

Two major administrative problems delayed our technical progress in FY-93. These problems were: (1) FY-93 funding for the USGS was not released by DOE until the end of FY-93, and (2) the process required for Geotech to gain formal approval from DOE to work with an industry partner was extremely slow. These two problems retarded technical work at the USGS and at RUST Geotech. Furthermore, the lack of experimental data, which were to have been provided to Los Alamos by those organizations to benchmark computer simulation codes, delayed the Los Alamos simulations while we sought and located an alternate source for benchmark data.

A third problem was that, although Los Alamos had the responsibility to coordinate this project, Los Alamos lacked the authority to affect the work being done by other organizations or to make any changes that could improve the progress of the project, other than the simulations. It is difficult to assess what impact this may have had on schedules and budgets, but it is clear that a more effective arrangement for coordinating the work was needed. (A new arrangement was agreed upon early in FY-94, with Jack Duray, a physicist and line manager at Geotech, accepting responsibility for coordinating the work).

APPENDIX B: MCNP INSTALLATION AND TESTING

The computer simulations for this project originally started on a network of Sun Sparc 2 workstations shared among users in the Geophysics group of the Earth and Environmental Sciences division at Los Alamos National Laboratory. The Sun network was upgraded during the summer of 1993 to about a dozen Sparc 2 and 10 workstations that are available on a time-shared basis, effectively giving us access to more than 50% of the CPU time. Additionally, an Hewlett-Packard 730 workstation was obtained at approximately the same time and is available to this project nearly full time.

The computer code(s) used for the simulations were installed and benchmarked with the standard package of 25 test problems distributed with the code on both the Sun and HP workstations. In addition, a number of problems previously run at DOE/Grand Junction by R. Wilson were run on both types of computers. The test problems and the problems from Grand Junction illustrated that the HP-730 workstation had over 4 times the speed of the Sun Sparc 2 workstations. This is primarily due to the capability of the HP-730 workstation to use dynamic memory, where the code uses as much internal memory (RAM) as possible at any given time, as well as the inherent differences in the processor speed. Dynamic memory use by the Sun Sparc 2 workstations actually increases the overall time used per problem. Real-time use of the HP-730 was even greater since it was solely used for these simulations and did not share CPU time with other users.

Due to the significant time benefits shown by the HP-730, we decided to upgrade the workstation to an HP-735 with a faster processor speed, and to upgrade the internal memory to 112 Mbytes from 32 Mbytes. This increased the speed of the computer simulations by another factor of 2, so that the HP-735 workstation is now the equivalent of over 8 Sun Sparc 2 workstations and about twice as fast as one processor in a Cray YMP for this software. In addition, we acquired essentially full-time access to another HP-735 workstation with 96 Mbytes of internal memory, bringing the computing power of the two HPs to the equivalent of over 16 Sun Sparc 2 workstations. The Sun network is still available for computer simulations and is used for running test problems, while the HP-735 computersre reserved for the final simulations which can take upwards of two weeks, or ~20,000 minutes, of computer time to obtain reasonable statistical accuracy.

In addition to the hardware upgrades, the computer code has been upgraded several times to include the latest features available such as color graphics. In each instance, the code is upgraded on all computers available and is tested against the standard set of test problems distributed with the code.